201-16554L

IUCLID

Data Set

Existing Chemical	:	ID: 68515-49-1
CAS No.	:	68515-49-1
EINECS Name	:	1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
EC No.	:	271-091-4
Molecular Weight	:	446
Structural Formula	:	c(ccc1C(=O)OCCC(C)CCC(C)CC)cc1C(=O)OCCC(C)CCC(C)CC
Molecular Formula	:	C2804H46

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	08.05.2006

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	08.05.2006
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	07.12.2006
Revision date	:	
Date of last update	:	07.12.2006
Number of pages	:	45
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes eleven CAS numbers (see Freetext).

Remark : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes the following eleven CAS numbers:

68648-93-1	1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)
117-84-0	1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)
16883-83-3	1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)
68515-40-2	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)
68515-45-7	1,2,-benzenedicarboxylic acid, dinonyl ester, branched and linear (DNP)
68515-43-5	1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)
84-77-5	1,2-benzenedicarboxylic acid, didecyl ester (DDP)
3648-20-2	1,2-benzenedicarboxylic acid, diundecyl ester (DUP)
85507-79-5	1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)
111381-91-0	1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)
68515-47-9	1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on

their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

22.06.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	> 99.7 % w/w
Colour	:	
Odour	:	
Remark	:	C9-C11 branched dialkyl ester, C10 rich.

22.06.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

2.1 MELTING POINT

Value	:	-46 °C
Decomposition	:	no, at °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Remark	:	Data are from a peer reviewed literature review of data from a variety of sources including manufacturer's data or handbook values.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Reliability	:	(2) valid with restrictions This robust summary is assigned a reliability of 2 because there is limited informtion on how the data were developed.
Flag	:	Critical study for SIDS endpoint

22.06.2006 (22)

Value	:	141 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI SuiteTM gives erroneously high results for the phthalate esters.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Reliability	:	(3) invalid

22.06.2006 (7)

2.2 BOILING POINT

Value	:	454 °C at 1013 hPa
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Reliability	:	(2) valid with restrictions

This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
23.06.2006 (7)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .0000000184 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisodecyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diisodecyl phthalate ester was 609.2 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
23.06.2006 (5)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	9.46 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisodecyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diisodecyl phthalate ester was 609.2 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

23.06.2006 (5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	.00004 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	

Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisodecyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for diisodecyl phthalate ester was 609.2 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
23.06.2006		(5)
Solubility in	:	
Value	:	< .00013 mg/l at 21 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: "Slow-Stir" Shake Flask
Year	:	
GLP	:	yes
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Remark	:	The procedure for this study involved adding TS to several

glass vessels containing 4 liters of carbon-treated well water to yield a nominal concentration of 100 mg/l. Each glass vessel contained a glass stir bar and was gently stirred with the aid of a stir plate. The TS which existed as a visible surface film of free product was allowed to equilibrate with the water in which it was in contact for a period of up to 9 days. After 3 and 9 days of equilibration, a 3 liter sample was removed from a port at the bottom of the vessel (thus minimizing sample contamination from free product on the surface) for DIDP analysis. Three test vessels were sampled in this manner at each time period in order to provide triplicate analyses for water solubility determination. Analyses first involved passing the aqueous sample through a solid phase extraction cartridge, eluting the cartridge with solvent, followed by subsequent concentration of the extract by solvent evaporation. This extract was then analyzed using GC/MS in the selective ion monitoring (SIM) mode. Special precautions were taken in this study to minimize laboratory contamination. Recoveries for samples spiked at 0.0006 mg/l were 97% using this procedure. Measured water solubilities for DIDP were below analytical detection limits that ranged from < 0.00003 to < 0.00013 mg/l.

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

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2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.00000000001895 cm³/(molecule*sec)
Degradation	:	50 % after 6.8 hour(s)
Deg. product	:	not measured
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark	:	50% degradation after 6.77 hrs or 0.56 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

23.06.2006 (7)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	3.4 year at 25 °C
t1/2 pH9	:	at °C
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Reliability	:	(2) valid with restrictions

This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
23.06.2006 (7)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	446.68
Temperature	25° C
Log Kow	9.46
Water Solubility	0.0000381 g/m3
Vapor Pressure	0.00000184 Pa
Melting Point	-46°C

Result : Using the Mackay Level I calculation, the following distribution is predicted for diisodecyl phthalate:

% Distribution	Compartment
0.0	Air
0.0	Water
97.7	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
23.06.2006 (17)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units

Molecular Weight	446.68
Temperature	25° C
Log Kow	9.46
Water Solubility	0.0000381 g/m3
Vapor Pressure	0.00000184 Pa
Melting Point	-46°C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	13.54a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from: Exxon Biomedical Sciences, Inc. (1995) and Boethling (2000):
Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result : Using the Mackay Level III calculation, the following distribution is predicted for diisodecyl phthalate:

Compartment	% Distribution
Air	1.0
Water	8.0
Soil	69.1
Sediment	21.9

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
23.06.2006 (17)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Contact time	:	28 day(s)
Degradation	:	= 67.1 (±) % after 28 day(s)
Result	:	readily biodegradable
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1994
GLP	:	no
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Result :

The biodegradation half-life <3 weeks. By day 28, 67.1% degradation of the test substance was observed. 10% biodegradation was achieved on approximately day 13, 50% biodegradation on approximately day 19, and >60% biodegradation on day 23.

By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. Oxygen uptake of the blanks were within guideline limits. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test substance as calculated using results of an elemental analysis of the test substance.

Test Substance:

Day	% Degradation*
12	4, 14, 11
13	11, 26, 20
14	20, 36, 27
23	48, 76, 57
28	57, 81, 64 (mean = 67.1)

Positive Reference Substance (Na Benzoate):

Day	% Degradation*
1	32, 36, 34
2	56, 66, 61
5	76, 89, 82

* replicate data

Test condition : Activated sludge and test medium were combined prior to test substance addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test substance was tested in triplicate, controls and blanks were tested in duplicate.

Test substance (1,2-benzenedicarboxylic acid, diiso-C10 alkyl esters) concentration was approximately 50 mg/L. The positive control (sodium benzoate) concentration was approximately 50 mg/L. Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars

and plates.

Test substance : 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich; CAS #68515-49-1
No information on purity, but believed to represent 100% commercial product.

Conclusion : The test substance is readily biodegradable.

Reliability : (1) valid without restriction
This summary is rated a "1" and represents a key study because it followed an OECD standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

Flag : Critical study for SIDS endpoint
23.06.2006 (8)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> .62
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	1975
GLP	:	yes
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Method : Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians.

Statistical methods-Moving average angle, Probit or Bionomial concentration.

Result : 96 hr LC50 >0.62 mg/L
Mean measured values were used in the LC50 calculation.

Nominal test concentrations: control, 0.094, 0.19, 0.38, 0.75, and 1.5 ul/L. Mean measured test concentrations: <0.021, 0.043, 0.075, 0.14, 0.25, and 0.62 mg/L.

Analytical samples were taken at time zero and on a composite of replicates at study termination. Measured values dropped slightly during the exposure period. Droplets of undissolved test material were observed on the surface of all test solutions throughout the exposure period and a film of undissolved test material was observed on the surface of the two high concentrations throughout the test.

% Mortality results at 96 hrs per replicate for control and treatment levels:

Conc. (mg/L)	Rep1/Rep2
Control	0 / 20
0.043	0 / 20
0.075	0 / 10
0.14	0 / 0
0.25	0 / 10
0.62	0 / 0

Test condition : Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15 L of solution. The diluter maintained a water turnover rate of 5 to 8 tank volumes per day. Two replicates of ten organisms were tested per treatment and control. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection.

Fish mean length = 62 mm and mean wet weight = 2.3 g. Test temperature = 11 Deg C. The pH ranged from 7.1 to 7.4. The mean dissolved oxygen ranged from 9.5 to 9.6 mg/L. Ranges of total hardness and alkalinity as CaCO3 of the dilution water were 20 to 26 mg/L and 14 to 22 mg/L, respectively.

Fish were obtained from a Montana supplier.

Test substance : Diisodecyl phthalate, (CAS# 68515-49-1)
(1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich)
Synonym: DIDP
Purity: 100% active ingredient

Conclusion : Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (1) valid without restriction
This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

Flag : Critical study for SIDS endpoint
23.06.2006 (6) (23)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : > .02
Analytical monitoring : yes
Method : other
Year : 1975
GLP : yes
Test substance : other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Method : Method/Guideline - U.S. EPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975.
Statistical methods incorporated the following procedures: Moving average angle, Probit, and Bionomial Probability.

Result : 48 hr EC50 >0.18 mg/L (based upon time zero analytical samples; no effects at test substance saturation). Value was recalculated as >0.02 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentrations: control, 0.16, 0.26, 0.43, 0.72, and 1.2 ul/L. Mean measured test concentrations of time 0 and 48 hr values: <0.014, 0.074, 0.12, 0.22, 0.34, and 0.61 mg/L.

Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined during study exposure. The high treatment solution is considered the maximum solubility achievable under the conditions of the test.

% Immobility results at 48 hrs per replicate for control and treatment levels in the first test:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 20
0.074	0 / 0 / 20
0.12	20 / 20 / 40

0.22	40 / 80 / 80
0.34	60 / 100 / 100
0.61	100 / 100 / 100

More than 50% of the organisms were trapped on the surface of all treatment solutions and a film of test material was present in all but the lowest treatment level. Consequently, the study was repeated as a limit test using a saturated treatment solution.

% Immobility results at 48 hrs per replicate for control and treatment levels in the second limit test:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 0
0.02	0 / 0 / 0

Undissolved test substance was avoided in the repeat study. Data from the second test are used to characterize the acute toxicity of the test substance.

Test condition : Test treatments for the initial test were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250 ml beakers with 200 ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).

Water quality parameters for the first test:
Test temperature = 21.5 +/- 0.5 Deg C. The pH was 8.4 at initiation and 8.4 on day 2. Dissolved oxygen ranged from 8.3 to 8.5 at initiation and 8.0 to 8.4 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Test treatments for the repeat study were prepared by mixing the test substance and 3 L of dilution water (fortified well water) on a magnetic stirrer for 1 hour at a loading of 9.7 mg/L, with a 50% vortex. After mixing the treatment solution was allowed to stand for 1 hour after which 2.5 L of solution was drained from the bottom of the flask into a glass bottle. The solution was allowed to stand for 24 hours after which 2.0 L was drained from the bottom into the test flasks and samples removed for analysis. Three replicates of five organisms were tested. Test vessels were 250 ml beakers with 200 ml of test solution. Control test vessels were prepared under the same conditions but without test substance. Analytical method was Gas Liquid Chromatography (GLC).

Water quality parameters for the second test:
Test temperature = 20 Deg C. The pH ranged from 7.9 to 8.0 at initiation and was 8.2 on day 2. Dissolved oxygen ranged from 7.6 to 8.4 at initiation and 8.4 to 8.5 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Test substance : Diisodecyl phthalate, (CAS# 68515-49-1)
(1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich)
Synonym: DIDP
Purity: unstated, but believed to be 100% active ingredient because the test material came from the same source as in the rainbow trout acute study.

Conclusion : Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability	:	(1) valid without restriction This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.
Flag	:	Critical study for SIDS endpoint

23.06.2006 (20) (23)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: biomass and growth rate
Exposure period	:	8 day(s)
Unit	:	mg/l
NOEC	:	= .8
EC50	:	> .8
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	1978
GLP	:	yes
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Method/Guideline - U.S. EPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978. Statistical methods - Moving average angle, Probit or Bionomial Test type - Static
Result	:	192 hr (8 day) EC50 >1.3 mg/L (based upon time zero analytical samples). Value was recalculated as >0.8 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997). Mean measured values were used in the final EC50 calculation. Nominal test concentration as a percent of a saturated solution: 0 (control) and 100.0%. Mean measured test concentrations of time 0 and 144 hr values: <0.10 and 0.8 mg/L (detection limit was 0.10 mg/L). Analytical samples taken at time zero and on a composite of replicates at termination. In-vivo chlorophyll a, measured until less than 5% change. Both cell number and in-vivo chlorophyll a, measured at termination. Control chlorophyll a or cell counts were not reported. A stimulatory effect of as compared with the control for chlorophyll a was measured on all sampling days after day 1. Analytical samples were taken at time zero and on a composite of replicates at termination. Chlorophyll a percent change relative to control on sampling days and cell number on day 8 results: Conc. Chlorophyll a percent change from control (mg/L) Day 1 Day 2 Day 4 Day 6 Day 8 Cell # Day 8 0.8 0 +2 +21 +23 +9 +2
Test condition	:	Algal Growth Medium was used as the control and diluent. 10 uL of test substance was added to 1.0 L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0 E4 cells/ml. Only one treatment level was evaluated (100% WSF) because earlier phthalate testing

suggested that toxic effects were not expected with higher molecular weight phthalate esters with low water solubility.

Lighting = 4,700 lux, Test temperature = 22+/-2 Deg C. The pH was 7.5 at initiation and 8.6 on day 8. Algal culture stock was obtained from University of Texas at Austin, TX.

Test substance : Diisodecyl phthalate, (CAS# 68515-49-1)
(1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich)
Synonym: DIDP
Purity: unstated, but believed to be 100% active ingredient as was provided in the rainbow trout study.

Conclusion : Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al (1997).

Reliability : (1) valid without restriction
The study procedure followed an accepted test guideline and applied GLP. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances. Control chlorophyll or cell counts not reported.

Flag : Critical study for SIDS endpoint
23.06.2006 (21) (23)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species : Oryzias latipes (Fish, fresh water)
Endpoint :
Exposure period : 284 day(s)
Unit :
Analytical monitoring : yes
Method : other
Year :
GLP : no
Test substance : other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Method : An Analysis of Variance (ANOVA) was used to determine differences in the groups based on survival, growth, and fecundity. The ANOVA was determined using the General Linear Models procedure of SAS.

Remark : Medaka were used because they are sensitive to estrogen and estrogenic compounds producing ovotestis and other reproductive effects. Medaka reach sexual maturity in 40 to 60 days post-hatch, which allows for a multigeneration study to be completed in one year.
The test substance was administered via the diet since this is the major route of exposure to hydrophobic compounds.

Result : The test diet was analyzed by GC-MS three times during the study (Pre-study, Day 136, and Day 284). Nominal loading was 20 µg/g. Mean test concentration of the test diet ranged from 19.2 ± 0.64 µg/g to 22.7 ± 0.81 µg/g.
No significant difference in survival was observed between the treated group and the controls.

Mean Percent Mortality

Generation	F0	F1	F2	
Control11.2	24.6	14.4		
Solvent Control		7.6	18.0	14.0

Test Substance	7.6	22.4 12.4

There were no treatment-related gross lesions or disease processes observed in the adult fish. No significant reduction growth or egg production was observed between the treated group and the controls. However, the untreated group produced fewer eggs than both the treated group and the solvent control group in both generations.
Sex ratio (male to female) was similar among all groups (approximately 1:1) for the F0, F1 and F2 generations. Phenotypic and histological gender classifications were in agreement for both males and females. T here was no statistically significant gonadal-somatic index (GSI) differences among the treated and control groups in either the F0 or the F1 generation.
F2 generation juvenile fish were processed on Day 42 post-hatch. The primary organs examined for general developmental conditions and the occurrence of lesions included the brain, digestive system, liver, kidney, gonads, and skeleton. There were no treatment-related histological lesions observed in the fish. The results demonstrate that the test substance did not elicit endocrine-mediated effects such as testis-ova, intersex conditions, or sex reversal in Japanese medaka.

EROD activity of the F1 generation male and female medaka were not significantly dofferent among the control and treated fish. Activity in male fish ranged from 0.04 to 0.08 pmol/min/mg protein and for female fish ranged from 0.09 to 0.12 pmol/min/mg protein. Significant induction or reduction in EROD activity was considered to be 2-fold different than the solvent control for either male or female hepatic samples. There were also no major metabolic differences among the groups with respect to testosterone hydroxylase activity. Hepatic vitellogenin production was not detectable in Western Blot analysis of F0 and F1 generation male medaka at 140 DPH. The F0 females showed faint banding at approximately 170 kDa and the F1 females showed a 2 to 3-fold increase in staining when compared to the untreated control group. Positive controls (17ß-estradiol) had a 5 to 6-fold increase in staining in both males and females when compared to the untreated control group.

Histological and biochemical endpoints are addressed in a separate peer-reviewed article "Patyna, P.J., et. al (2004) Dietary Diisononyl Phthalate and Diisodecyl Phthalate Exposure in the Japanese Medaka (Oryzias latipes) Multigeneration Assay, submitted to Ecotox and Env. Safety."

Test condition : Diet Prep:
A single dietary concentration was prepared at a nominal loading of 20 µg/g. The exposure concentration represented a reasonable worst-case scenario based on USEPA field measurements and equilibrium partitioning theory predictions for concentrations in prey organisms. The experimental diet was prepared by adding the test substance to Tetramin flake fish food (5% lipid content) with the help of acetone as a solvent in order to evenly distribute the test substance in the fish food. The solvent was allowed to evaporate overnight under ambient laboratory conditions. An acetone solvent control was included with an untreated control group and prepared under similar conditions. The diets were stored at -20°C ± 2°C for the duration of the study to prevent spoilage. The feed was analyzed by GC-MSD for concentration verification purposes prior to, during, and after the study.

Methods:
A flow-through exposure system was constructed to provide a sufficient volume of water to the exposure chambers. The flow rate (approximately 250 ml/min) was monitored daily and adjusted as necessary in order to maintain optimal water quality for the test organisms.
Five replicate chambers were prepared for each of the three treatment groups (treated, solvent control, untreated control). Test chambers were 19 liter glass aquaria with stainless steel standpipes cut to allow a test

volume of 10 liters of water. Embryos collected during the study were hatched in 250 ml glass beakers under continuous aeration.
Test water in the hatching chambers was replaced as needed to preserve water quality and maintain embryo health. During overlap between generations, juvenile fish were housed in glass cylinders suspended in the test chambers to prevent losses due to consumption by adult fish.
Replicate integrity was maintained throughout the study.
Temperature was measured daily in each replicate chamber and was maintained at 25°C ± 2°C for the duration of the study. Dissolved oxygen and pH were measured at least twice per week in one replicate chamber of each group. Ranges during the study were:

	Untreated Control	Acetone Control	Test Substance
Dissolved Oxygen (mg/l)	7.0-8.8	7.1-8.7	6.8-8.8
pH	6.5-7.6	6.9-7.7	6.8-7.7

For the F0 generation, 50 medaka larvae per replicate (a total of 250 fish per group) were fed the appropriate diet at a rate of 50% body weight per day. The food ration was periodically adjusted to compensate for growth of the fish during the study. Feeding was also supplemented three times weekly with freshly hatched brine shrimp (Artemia spp.).

Observations for mortality were performed and recorded daily. Dead organisms were recorded and removed from the test chambers. Test chambers were also cleaned periodically to remove accumulated organic material. Once adults reached sexual maturity (about 40 to 60 days post-hatch (DPH)), eggs were collected on sponge filters. Egg production was observed for approximately 3 to 4 weeks and recorded before eggs were collected for hatching of the next generation. Eggs for hatching were collected once all replicates were observed producing eggs. During the embryo-rearing stages of the study the rearing chambers were observed daily and all embryos with fungus or an opaque appearance were removed. Eggs from each replicate were hatched to provide 50 larval fish for the next generation. The remaining collected eggs were counted and frozen for chemical analysis. At termination of each generation (140 DPH) there remained at least 25 fish per replicate (125 fish per group). Population, individual, and biochemical test parameters were evaluated at this time. Male and female fish were processed separately. Fish were evaluated for morphometric parameters such as total weight, standard length, gonad weight, and gonadal-somatic index.

As with the original population (F0), the F1 fish were allowed to spawn (F2 generation) and fecundity, egg viability, and embryo development were evaluated. Adult F1 fish were also evaluated based on histopathology, morphological characteristics, and biochemical parameters. F1 larvae were evaluated for lesion occurrence, stage development, post-hatch survival and growth. The F2 larvae were allowed to grow out until 42 DPH, at which time they were weighed, measured, and processed for histopathology evaluation.

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Conclusion : The test substance did not produce significant carcinogenic, teratological, or reproductive effects on either the original population or subsequent generations.

Reliability : (2) valid with restrictions
Specific guidelines for the study were not available. The study was performed following procedures outlined in existing chronic fish toxicity test guidelines.

Flag : Critical study for SIDS endpoint
07.12.2006

(12)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia magna (Crustacea)
Endpoint	:	reproduction rate
Exposure period	:	21 day(s)
Unit	:	mg/l
NOEC	:	= 1
EC50	:	> 1
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year	:	1984
GLP	:	yes
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	The test method followed the Daphnid chronic testing procedure described in OECD guideline 202 (1984) with the use of a dispersant, castor oil 40-ethoxylate (Marlowet 40), in accordance with guideline specifications.
Result	:	Daphnia parent (Po) survival, reproduction (cumulative number of offspring, F1, per live parent), and parent length were evaluated as the biological endpoints. Diisodecyl phthalate ester showed no effect on survival, reproduction, and length at a loading of 1.0 mg/L test substance and 10 mg/L dispersant under the conditions of this test.

	Po % Mortality	Mean F1/Surviving Po	Po Mean Length
Test Substance	10	105 (sd=7)	4.2 (sd=0.12)
Control	0	93 (sd=9)	4.1 (sd=0.17)

Test condition : Test substance exposure solutions were prepared using stock dispersions prepared by adding 100 mg substance and 1000 mg dispersant (castor oil 40-ethoxylate; Marlowet 40), then bringing the test solution to 1 L by adding dilution medium. The dilution medium was Elendt's medium (Elendt and Bias, 1990), which was pH adjusted to 8 and aerated for >2 hours prior to use.

Ten replicate test systems with 1 daphnid each (< 24 hours old) were prepared in glass beakers with loose fitting lids. Each beaker contained 80 ml of exposure solution with a depth of approximately 5 cm. The photoperiod was controlled to 16 hours light and 8 hours dark with a 15 minute transition period.

The exposure solution was renewed every Monday, Wednesday, and Friday. On each renewal day the parent organism (Po) was transferred to a new exposure solution and neonates (F1) were counted. Water quality measurements including dissolved oxygen concentration and pH were determined at every renewal for the new and old exposure and control solutions. Test conditions were:

Temperature = 20 +/- 1.0 degree C
Water harness = >140 mg/L (as CaCO3)
Alkalinity = >100 mg/L (as CaCO3)
pH = approximately 8
Dissolved oxygen = 8-9 mg/L

Standard daily feeding rates with the cultured alga, Chlorella vulgaris, was supplemented with microencapsulated food, "Frippak Booster".

Test substance analyses of new and old exposure solutions were performed using gas chromatography with flame ionization detection, after a hexane extraction. The mean measured test substance concentrations were 1.0 mg/L in new exposure solutions and 1.0 mg/L in old exposure

solutions, which represents 100 and 100%, respectively, of the nominally added test substance.

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Conclusion : Chronic invertebrate (Daphnia magna) toxicity data reported for diisodecyl phthalate ester are consistent with valid data for several high molecular weight phthalate esters as summarized by Brown et al. (1998), Staples et al. (1997), and Rhodes et al. (1995). These data show that high molecular weight phthalate esters, including diisodecyl phthalate ester, do not produce chronic toxicity to Daphnia magna. Testing was conducted at a loading that exceeds the water solubility of diisodecyl phthalate ester (0.61 ug/L; Letinski et al., 2002) after it was demonstrated that such a procedure was able to satisfactorily disperse the test substance and that it prevented floatation of the test organism, a documented problem that can occur when evaluating the toxicity of similar substances.

Reliability : (1) valid without restriction
The study proceedure followed an accepted test guideline and applied GLP. The study procedure and results were accepted in a peer reviewed journal. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag : Critical study for SIDS endpoint
07.12.2006 (2)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

Species : other: Chironomus tentans
Endpoint : other: mortality and growth
Exposure period : 14 other: day(s)
Unit : other: mg/kg sediment dw
NOEC : = 2630
LC50 : > 2630
Method : other: US Environmental Protection Agency. Methods for measuring the toxicity and bioaccumulation of sediment-associated contaminants with freshwater invertebrates. EPA/600/R-94/024
Year : 1994
GLP : yes
Test substance : other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Remark : LL0: m = 3000
LL50: m > 3000

Result : Chironomus tentans survival and growth were evaluated as the biological endpoints. The test substance showed no effect on survival or growth at a test substance loading of 3000 mg/kg sediment dry weight.

There were five control and five exposure systems each containing 10 organisms and two sand controls with 10 organisms each. The means (ranges) of test substance concentrations in pore water and bulk sediment, and mean number of survivors (mean orgnaism dry weights) were as follows:
Pore water: control mean conc. = <0.004 mg/L (<0.004-0.004), exposure mean conc. = 1.18 mg/L (0.766-1.80);
Bulk sediment: control conc. = <1.89 mg/kg sediment dry weight (<1.89-<1.89), exposure mean conc. = 2630 mg/kg sediment dry weight (2340-3320)
Control survivors = 47 (1.60 mg dry weight)
Exposure survivors = 45 (1.77 mg dry weight)
Sand survivors = 18 (0.99 mg dry weight)

Although the test substance was not tested for stability, it was assumed

from the measured half-lives of DHP (di-n-hexyl phthalate) and DIDP (diisodecyl phthalate, this substance) and the apparent stability of DEHP (diehthylhexyl phthalate) that the test substance would be sufficiently stable to conduct toxicity tests (DHP and DEHP were also evaluated in this study). DEHP was recently reported to have a half-life of <15 d in aqueous solution but >70 d in soil. Overall, the results from the stability study indicated that the high molecular weight phthalate esters were sufficiently stable to proceed with 10-day sediment toxicity tests.

Test condition : Sediment Sources and Characteristics

Uncontaminated, natural sediment samples for this study were collected from Airport Pond (St. Louis County, MN, USA) and West Bearskin Lake (Cook County, MN, USA). Samples were collected with a Ponar dredge, placed into clean polyethylene containers, and stored at 4 degrees C until used. For the test, the sediments were homogenized in a 119-L stainless steel container using a commercial drill with a stainless steel mortar-mixing paddle. To achieve a desired medium total organic carbon (TOC) sediment level, aliquots from Airport Pond and West Bearskin Lake were blended. A summary of TOC content and particle size distribution for the two blended sediments follows (+/- standard deviation in parentheses): the mean TOC content was 4.8% (0.65) ; sand content was 46.9% (4.09); silt content was 30.2% (3.59); coarse clay content was 2.3% (1.47); and fine clay content was 20.5% (1.86).

Amendment of Sediment with Test Substance

The test substance was dissolved in acetone and coated onto a 20% aliquot of a wet sediment sample. The sediment aliquot was dried and then placed into a 4-L glass jar, which was rotated in an air stream to evaporate the acetone. Deionized water equal to the volume lost in drying the 20% portion of wet sediment was then added to the dried sediment aliquot, mixed, and added back into the jar containing the remaining 80% wet sediment sample. The jar was sealed with a Teflont-lined cap and rotated on a roller mill in a cold room (approximately 4 degrees C) for approximately 6 days at a speed of approximately 8 rpm.

During mixing, samples of sediment were collected at periodic intervals for analysis of PE concentrations in the bulk sediment and pore water. Homogeneity of mixing was determined from multiple sediment samples usually collected on day 6. The degree to which an equilibrium in pore-water concentrations had been achieved was determined from samples of pore water collected on two occasions, usually days 3 and 6.

Sediment Testing

Sediment testing proceeded in two phases.

The first phase evaluated the effectiveness of the mixing process in achieving a homogeneous distribution of test substance in bulk sediment, the establishment of equilibrium concentrations of test chemicals in the pore water, and the stability of the test substance in pore water under simulated toxicity test conditions. This phase was used to determine, in part, if meaningful toxicity tests could be performed (i.e., to assess if stable exposure concentrations could be maintained during the test period). The second phase evaluated the toxicity of the test substance in spiked sediments toward the test species.

During the mixing process, samples of bulk sediment were collected on days 1, 3, and 6 after test substance amendment and pore water samples were separated by centrifugation. Duplicate bulk sediment samples were analyzed on day 6 to evaluate homogeneity. Mean pore-water concentrations were compared between days 3 and 6 to determine the

extent to which equilibrium had been achieved. Approximately 100 ml of test substance-amended wet sediment was then transferred into 300-ml high-form beakers and placed into the toxicity testing system described below. Samples of sediment, overlying water, and pore water were collected at intervals over 9 to 10 days. The PE stability in pore water was evaluated by calculating half-lives, using log-transformed concentrations in simple linear regression analyses with time. Five replicates of a single nominal concentration of 3,000 mg/kg dry sediment and five control replicates were used to enhance statistical resolution.

The rationale for a spiking limit of 3,000 mg/kg was based on several factors. First, the application of true water solubility limits for di-n-hexyl phthalate (DHP) and diethylhexyl phthalate (DEHP) of 0.05 and 0.003 mg/L in EqP calculations resulted in sediment spiking limits of approximately 2,400 and 1,700 mg/kg, respectively, for a low TOC sediment. Second, the sediment concentration of 3,000 mg/kg is well in excess of environmental exposures since it exceeds by at least two orders of magnitude recently reported field concentrations of DEHP as well as maxima for any of the other high molecular weight PEs. Third, preliminary experiments at a DEHP spiking level of 30,000 mg/kg appeared to adversely affect the dissolved oxygen concentration. Based on published aquatic toxicity data and water-only toxicity test results (Call et al., 2001b), the target dose of 3,000 mg/kg dry sediment was not anticipated to exhibit acute toxicity.

For the second phase (i.e., toxicity testing), 100 ml of test substance-amended test sediment was added to each beaker and allowed to equilibrate in the flow-through test system for approximately 24 hours before test organisms were added. Ten Hyalella azteca (7-14 days old) or ten Chironomus tentans larvae (2nd-3rd instars, 10-12 days old) were then added to each exposure beaker. The daily feeding regimes utilized for the chambers containing H. azteca and C. tentans consisted of 1.0 to 1.5 ml of a yeast-trout chow-Cerophyllt mixture and 1.5 ml of a 4 g/L Tetrafint slurry (TetraWerke, Melle, Germany), respectively. Tests were conducted in an intermittent water renewal system, with screened 300-ml high-form beakers as the primary exposure chambers. They were conducted at a nominal temperature of 23 degrees C, with a 16:8 light:dark photoperiod. The beakers contained approximately 100 ml of sediment and 100 to 175 ml of overlying water, dependent on the stage in the siphoning and renewal cycle. Overlying water, was replaced at a rate of four to eight volume additions daily. The water in the tanks holding the primary exposure chambers was aerated throughout the exposure period to ensure that an adequate level of dissolved oxygen was maintained. General observations were made daily, with counts of survivors obtained after the 10-day exposure period. At that time, the sediment was sieved, survivors collected, cleaned of debris, oven-dried for approximately 24 hours at 105 degrees C, and weighed. Weights were determined to 0.01 mg for the pooled survivors from each replicate.

Toxicity tests (48 hours) with KCl as a reference toxicant were performed regularly throughout the testing program with the test species to ensure that organisms used in tests were healthy and that LC50 values were within acceptable limits for performing the toxicity tests. The reference toxicant tests were conducted within one month of the test substance toxicity test. Control animal survival acceptability criteria of 80 and 70% were used for 10-day toxicity tests with H. azteca and C. tentans, respectively. A silica sand performance control also accompanied each toxicity test as a check on the performance of animals in the test system. Tests were performed using documentation consistent with good laboratory practices.

Temperature, dissolved oxygen, and pH were recorded in all test chambers on days 0 and 10. Conductivity was measured in all test chambers on days

1 and 9. Hardness, alkalinity, and ammonia were measured on days 1 and 9 in at least one sediment control chamber. On days 2 to 9, temperature, dissolved oxygen, and pH were measured in at least one sediment control chamber and one exposure chamber.

Test Substance Analyses

Samples of bulk sediment, pore water, and overlying water were sampled on days 0 and 10 and at two intermediate times for measurement of test substance concentrations. Overlying water samples (500 ml) were collected with an Eppendorf pipettor approximately 1 to 2 cm above the sediment. Samples were analyzed by high performance liquid chromatography. The overlying water was then siphoned out of the beaker to obtain sediment samples. Sediment cores were collected using a glass tube (13-mm inner diameter). Pore water was defined as the supernatant liquid obtained from centrifuging wet sediment at 10,000 g for 30 minutes. Following centrifugation, an aliquot of the pore water was pipetted into a vial and a 1:1 mixture of acetonitrile and deionized water added to bring the sample volume to 1 ml. The vial was capped and mixed, after which the contents were centrifuged to remove any precipitate present. The remainder of the pore water was removed from the sample tube and the weight of the bulk sediment was determined. Sediments were extracted by adding 5 ml of acetonitrile to the centrifuged pellet (from the pore-water preparation step), mixing the pellet and acetonitrile with a stainless steel spatula, and sonicating for 15 minutes in a 35 degrees C water bath. Samples were mixed with a clean spatula and then sonicated for an additional 15 minutes. The tube was centrifuged in a bench-top centrifuge for 5 minutes and a sample of the supernatant diluted with a mixture of acetonitrile and water (1:1, v/v). The remaining supernatant was removed from the sediment and the sediment dried overnight at 27 degrees C for dry weight (%) estimates.

The test substance concentrations in aqueous and sediment samples were measured by high performance liquid chromatography using Shimadzu and Gilson instruments containing columns of either Lichrospher 100 RP-18 or Lichrospher 100 CN (EM Science, Gibbstown, NJ, USA). Detector wavelengths of 274 and 224 nm were employed, and eluent mixtures were acetonitrile and water.

Analytical standards bracketing the predicted test substance concentrations being analyzed were prepared in acetonitrile and diluted with deionized water. Samples were routinely checked for spike recoveries and repeatability of duplicate analyses.

Statistical Analysis

Survival data from toxicity tests were summarized using the trimmed Spearman-Karber method. Dry weight data were analyzed by one-way analysis of variance and Dunnett's procedure using a SigmaStatt Program (SPSS, Chicago, IL, USA).

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich; purity = 99.7%; commercial grade

Conclusion : The sediment toxicity data for Chironomus tentans reported for diisodecyl phthalate ester (DIDP) are consistent with the sediment and aqueous exposure toxicity data data for several high molecular weight phthalate esters for three freshwater invertebrates as summarized by Call et al. (2001a, 2001b). These data clearly showed that high molecular weight phthalate esters, including DIDP, did not produce toxicity, as measured by survival rate and growth, to freshwater sediment invertebrates at sediment loading rates that far exceed expected field levels, based on field measurements of similar higher molecular weight phthalate esters.

Reliability : (1) valid without restriction

The study proceedure followed an accepted test guideline and applied GLP. The study procedure and results were accepted in a peer reviewed journal. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag : Critical study for SIDS endpoint
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Species : other: Hyalella azteca
Endpoint : other: mortality and growth
Exposure period : 14 other: day(s)
Unit : other: mg/kg sediment dw
NOEC : = 2090
LC50 : > 2090
Method : other: US Environmental Protection Agency. Methods for measuring the toxicity and bioaccumulation of sediment-associated contaminants with freshwater invertebrates. EPA/600/R-94/024
Year : 1994
GLP : yes
Test substance : other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Remark : LL0: m = 3000
LL50: m > 3000

Result : Hyalella azteca survival and growth were evaluated as the biological endpoints. The test substance showed no effect on survival or growth at a test substance loading of 3000 mg/kg sediment dry weight.

There were five control and five exposure systems each containing 10 organisms and two sand controls with 10 organisms each. The means (ranges) of test substance concentrations in pore water and bulk sediment, and mean number of survivors (mean orgnaism dry weights) were as follows:
Pore water: control mean conc. = <0.047 mg/L (<0.004-0.110), exposure mean conc. = 0.931 mg/L (0.376-2.00);
Bulk sediment: control conc. = <1.89 mg/kg sediment dry weight (<1.89-<1.89), exposure mean conc. = 2090 mg/kg sediment dry weight (1550-2630)
Control survivors = 49 (0.15 mg dry weight)
Exposure survivors = 50 (0.16 mg dry weight)
Sand survivors = 20 (0.12 mg dry weight)

Although the test substance was not tested for stability, it was assumed from the measured half-lives of DHP (di-n-hexyl phthalate) and DIDP (diisononyl phthalate, this substance) and the apparent stability of DEHP (diehthylhexyl phthalate) that the test substance would be sufficiently stable to conduct toxicity tests (DHP and DEHP were also evaluated in this study). DEHP was recently reported to have a half-life of <15 d in aqueous solution but >70 d in soil. Overall, the results from the stability study indicated that the high molecular weight phthalate esters were sufficiently stable to proceed with 10-day sediment toxicity tests.

Test condition : Sediment Sources and Characteristics

Uncontaminated, natural sediment samples for this study were collected from Airport Pond (St. Louis County, MN, USA) and West Bearskin Lake (Cook County, MN, USA). Samples were collected with a Ponar dredge, placed into clean polyethylene containers, and stored at 4 degrees C until used. For the test, the sediments were homogenized in a 119-L stainless steel container using a commercial drill with a stainless steel mortar-mixing paddle. To achieve a desired medium total organic carbon (TOC) sediment level, aliquots from Airport Pond and West Bearskin Lake were blended. A summary of TOC content and particle size distribution for the two blended sediments follows (+/- standard deviation in parentheses): the mean TOC

content was 4.8% (0.65); sand content was 46.9% (4.09); silt content was 30.2% (3.59); coarse clay content was 2.3% (1.47); and fine clay content was 20.5% (1.86).

Amendment of Sediment with Test Substance

The test substance was dissolved in acetone and coated onto a 20% aliquot of a wet sediment sample. The sediment aliquot was dried and then placed into a 4-L glass jar, which was rotated in an air stream to evaporate the acetone. Deionized water equal to the volume lost in drying the 20% portion of wet sediment was then added to the dried sediment aliquot, mixed, and added back into the jar containing the remaining 80% wet sediment sample. The jar was sealed with a Teflont-lined cap and rotated on a roller mill in a cold room (approximately 4 degrees C) for approximately 6 days at a speed of approximately 8 rpm.

During mixing, samples of sediment were collected at periodic intervals for analysis of PE concentrations in the bulk sediment and pore water. Homogeneity of mixing was determined from multiple sediment samples usually collected on day 6. The degree to which an equilibrium in pore-water concentrations had been achieved was determined from samples of pore water collected on two occasions, usually days 3 and 6.

Sediment Testing

Sediment testing proceeded in two phases.

The first phase evaluated the effectiveness of the mixing process in achieving a homogeneous distribution of test substance in bulk sediment, the establishment of equilibrium concentrations of test chemicals in the pore water, and the stability of the test substance in pore water under simulated toxicity test conditions. This phase was used to determine, in part, if meaningful toxicity tests could be performed (i.e., to assess if stable exposure concentrations could be maintained during the test period). The second phase evaluated the toxicity of the test substance in spiked sediments toward the test species.

During the mixing process, samples of bulk sediment were collected on days 1, 3, and 6 after test substance amendment and pore water samples were separated by centrifugation. Duplicate bulk sediment samples were analyzed on day 6 to evaluate homogeneity. Mean pore-water concentrations were compared between days 3 and 6 to determine the extent to which equilibrium had been achieved. Approximately 100 ml of test substance-amended wet sediment was then transferred into 300-ml high-form beakers and placed into the toxicity testing system described below. Samples of sediment, overlying water, and pore water were collected at intervals over 9 to 10 days. The PE stability in pore water was evaluated by calculating half-lives, using log-transformed concentrations in simple linear regression analyses with time. Five replicates of a single nominal concentration of 3,000 mg/kg dry sediment and five control replicates were used to enhance statistical resolution.

The rationale for a spiking limit of 3,000 mg/kg was based on several factors. First, the application of true water solubility limits for di-n-hexyl phthalate (DHP) and diethylhexyl phthalate (DEHP) of 0.05 and 0.003 mg/L in EqP calculations resulted in sediment spiking limits of approximately 2,400 and 1,700 mg/kg, respectively, for a low TOC sediment. Second, the sediment concentration of 3,000 mg/kg is well in excess of environmental exposures since it exceeds by at least two orders of magnitude recently reported field concentrations of DEHP as well as maxima for any of the other high molecular weight PEs. Third, preliminary experiments at a DEHP spiking level of 30,000 mg/kg appeared to adversely affect the dissolved

oxygen concentration. Based on published aquatic toxicity data and water-only toxicity test results (Call et al., 2001b), the target dose of 3,000 mg/kg dry sediment was not anticipated to exhibit acute toxicity.

For the second phase (i.e., toxicity testing), 100 ml of test substance-amended test sediment was added to each beaker and allowed to equilibrate in the flow-through test system for approximately 24 hours before test organisms were added. Ten Hyalella azteca (7-14 days old) or ten Chironomus tentans larvae (2nd-3rd instars, 10-12 days old) were then added to each exposure beaker. The daily feeding regimes utilized for the chambers containing H. azteca and C. tentans consisted of 1.0 to 1.5 ml of a yeast-trout chow-Cerophyllt mixture and 1.5 ml of a 4 g/L Tetrafint slurry (TetraWerke, Melle, Germany), respectively. Tests were conducted in an intermittent water renewal system, with screened 300-ml high-form beakers as the primary exposure chambers. They were conducted at a nominal temperature of 23 degrees C, with a 16:8 light:dark photoperiod. The beakers contained approximately 100 ml of sediment and 100 to 175 ml of overlying water, dependent on the stage in the siphoning and renewal cycle. Overlying water, was replaced at a rate of four to eight volume additions daily. The water in the tanks holding the primary exposure chambers was aerated throughout the exposure period to ensure that an adequate level of dissolved oxygen was maintained. General observations were made daily, with counts of survivors obtained after the 10-day exposure period. At that time, the sediment was sieved, survivors collected, cleaned of debris, oven-dried for approximately 24 hours at 105 degrees C, and weighed. Weights were determined to 0.01 mg for the pooled survivors from each replicate.

Toxicity tests (48 hours) with KCl as a reference toxicant were performed regularly throughout the testing program with the test species to ensure that organisms used in tests were healthy and that LC50 values were within acceptable limits for performing the toxicity tests. The reference toxicant tests were conducted within one month of the test substance toxicity test. Control animal survival acceptability criteria of 80 and 70% were used for 10-day toxicity tests with H. azteca and C. tentans, respectively. A silica sand performance control also accompanied each toxicity test as a check on the performance of animals in the test system. Tests were performed using documentation consistent with good laboratory practices.

Temperature, dissolved oxygen, and pH were recorded in all test chambers on days 0 and 10. Conductivity was measured in all test chambers on days 1 and 9. Hardness, alkalinity, and ammonia were measured on days 1 and 9 in at least one sediment control chamber. On days 2 to 9, temperature, dissolved oxygen, and pH were measured in at least one sediment control chamber and one exposure chamber.

Test Substance Analyses

Samples of bulk sediment, pore water, and overlying water were sampled on days 0 and 10 and at two intermediate times for measurement of test substance concentrations. Overlying water samples (500 ml) were collected with an Eppendorf pipettor approximately 1 to 2 cm above the sediment. Samples were analyzed by high performance liquid chromatography. The overlying water was then siphoned out of the beaker to obtain sediment samples. Sediment cores were collected using a glass tube (13-mm inner diameter). Pore water was defined as the supernatant liquid obtained from centrifuging wet sediment at 10,000 g for 30 minutes. Following centrifugation, an aliquot of the pore water was pipetted into a vial and a 1:1 mixture of acetonitrile and deionized water added to bring the sample volume to 1 ml. The vial was capped and mixed, after which the contents were centrifuged to remove any precipitate present. The

remainder of the pore water was removed from the sample tube and the weight of the bulk sediment was determined. Sediments were extracted by adding 5 ml of acetonitrile to the centrifuged pellet (from the pore-water preparation step), mixing the pellet and acetonitrile with a stainless steel spatula, and sonicating for 15 minutes in a 35 degrees C water bath. Samples were mixed with a clean spatula and then sonicated for an additional 15 minutes. The tube was centrifuged in a bench-top centrifuge for 5 minutes and a sample of the supernatant diluted with a mixture of acetonitrile and water (1:1, v/v). The remaining supernatant was removed from the sediment and the sediment dried overnight at 27 degrees C for dry weight (%) estimates.

The test substance concentrations in aqueous and sediment samples were measured by high performance liquid chromatography using Shimadzu and Gilson instruments containing columns of either Lichrospher 100 RP-18 or Lichrospher 100 CN (EM Science, Gibbstown, NJ, USA). Detector wavelengths of 274 and 224 nm were employed, and eluent mixtures were acetonitrile and water.

Analytical standards bracketing the predicted test substance concentrations being analyzed were prepared in acetonitrile and diluted with deionized water. Samples were routinely checked for spike recoveries and repeatability of duplicate analyses.

Statistical Analysis

Survival data from toxicity tests were summarized using the trimmed Spearman-Karber method. Dry weight data were analyzed by one-way analysis of variance and Dunnett's procedure using a SigmaStatt Program (SPSS, Chicago, IL, USA).

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich; purity = 99.7%; commercial grade

Conclusion : The sediment toxicity data for Hyalella azteca reported for diisodecyl phthalate ester (DIDP) are consistent with the sediment and aqueous exposure toxicity data data for several high molecular weight phthalate esters for three freshwater invertebrates as summarized by Call et al. (2001a, 2001b). These data clearly showed that high molecular weight phthalate esters, including DIDP, did not produce toxicity, as measured by survival rate and growth, to freshwater sediment invertebrates at sediment loading rates that far exceed expected field levels, based on field measurements of similar higher molecular weight phthalate esters.

Reliability : (1) valid without restriction
The study proceedure followed an accepted test guideline and applied GLP. The study procedure and results were accepted in a peer reviewed journal. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag : Critical study for SIDS endpoint
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4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species	:	Lactuca sativa (Dicotyledon)
Endpoint	:	other: germination
Exposure period	:	5 day(s)
Unit	:	mg/kg soil dw
NOEC	:	= 8630
LC50	:	> 8630
Method	:	other: U.S. EPA-600/3-88/029
Year	:	1996
GLP	:	yes

Test substance : other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Method : Statistical Method: Dunnett's Procedure (on tailed T test), SAS

Result : Seed germination (mean % germinated) in the controls met guideline requirements, which validates the test results.

Soil samples loaded at 10,000 mg test substance/kg soil were analyzed for DIDP. The soil analytical results are based on the mean of duplicate samples for each soil sampled:

Soil Sample	DIDP Conc. Day -1 (mg/kg soil, dry wt.)
Snyder Soil	8630
Artificial Soil	8551

DIDP demonstrated no effect on germination in the two soils tested at a soil loading of 10,000 mg/kg soil (dry wt.). The following are the germination results:

Soil Sample	Number Seeds Germinated*	Mean % Germinated
Snyder Soil Control		
Lettuce	39,36,39,38,35	94
Ryegrass	34,40,34,33,40	91
Artificial Soil Control		
Lettuce	39,40,40,40,35	97
Ryegrass	38,38,38,38,35	94
Snyder Soil + DIDP		
Lettuce	33,40,31,32,35	86
Ryegrass	40,39,38,37,40	97
Artificial Soil + DIDP		
Lettuce	40,37,40,37,39	97
Ryegrass	38,38,38,37,38	95

*40 seeds were added per replicate. There were five replicates per control and treatment.

Test condition : Two soils were tested, a natural soil and an artificial soil. Natural soil was obtained from Snyder Research Farm located in Pittstown, NJ, USA, which was managed by Rutgers University. The soil was sieved through a 10 mesh sieve prior to use to remove large particles. Artificial soil was prepared using 70% sand, 20% clay, and 10% peat.

Seeds were inspected and sized. Lettuce seeds selected for the test passed through a 1/6 x 1/30 inch screen. Ryegrass seeds selected for the test passed through a 1/6 x 1/28 inch screen.

Test soils were homogenized prior to use by placing soil into 4L size plastic (HDPE) containers and mixing on a jar mill for approximately 15 minutes. After homogenizing, a sample was removed to determine the moisture fraction. The moisture fraction was measured by placing soil into a crystallizing dish and weighing it (initial wt.). The sample and crystallizing dish were then placed in an oven at 100C for 23 hours. After drying and cooling in a desiccator, the final weight of the sample and crystallizing dish was measured.

The water holding capacity of each soil was determined as follows: 25g of

the dried sample was placed into a 100mL glass beaker with 25mL of reverse osmosis water and mixed thoroughly. This slurry was added to a pre-weighed, wetted filter paper and funnel (initial weight = wt. of funnel, wetted paper, + 25 g soil). The filter paper (#113 Whatman 150mm) was wetted with 9mL of reverse osmosis water. The glass funnel measured 10cm top diameter with an approximately 30mm stem. The slurry, filter and funnel were covered with aluminum foil and allowed to stand for 3 hours at which time a final weight was measured. The water holding capacity, expressed in mL water/100g of soil, is the difference between the final and initial weights multiplied by 4 to achieve 100g equivalence.

The test chambers were bottom halves of 150mm (diameter) x 15mm (high) plastic petri dishes placed in approximately 11" x 11" Ziploc bags. Each dish contained approximately 190g of test soil including the cover soil.

Soil treatments included: control (no test material) and 10,000 mg DINP per kg soil (dry wt.). Soil was hydrated at 85% of water holding capacity. Five replicates each of the two soils were tested, each with a control soil.

Two plant species were tested, lettuce (Lactuca sativa) and ryegrass (Lolium sp.).

Prior to seed distribution, all treatment replicates were randomly positioned, then 40 seeds were distributed to each chamber. The seeds were distributed about the surface, but not closer than approximately 0.5 inches from the edge of the test chamber. Approximately 90g of cover soil was then evenly distributed on top of each hydrated treatment and control soils. Each chamber was placed directly into a resealable polypropylene (Ziploc) bag, centered over the bottom of the bag. The sides were raised to a vertical position over the chamber and the plastic covers were removed. The bags were then sealed leaving headspace.

Test temperature: 24.5C (sd = 0.3C), as measured continuously and recorded by computer. Test Photoperiod: Initial 48 hours dark, followed by 16 hours of light and 8 hours of dark until termination of the test. Light intensity ranged from 4300+/- 430 Lux during daylight periods (measured daily).

Soil pH was measured at test initiation (day 0) of the study. Ten grams of each treatment were mixed with 20mL of distilled water. The pH value of the slurry was measured using a soil pH probe. Soil pH ranged from 6.4 to 7.0.

At test termination, after 120 hrs of exposure, the number of germinated seeds in each dish was determined by counting each seedling that protruded above the surface of the soil.

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich. No information on purity, but believed to be 100% commercial product.

Conclusion : Diisodecyl phthalate ester did not significantly effect the germination of lettuce and ryegrass seeds at a very high test material/soil loading.

Reliability : (1) valid without restriction
The study was conducted according to the test guideline and there were no significant deviations to the guideline that would suggest the results were questionable. Therefore the study was assessed as valid.

Flag : Critical study for SIDS endpoint
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4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	other: Earthworm Acute Toxicity Test
Species	:	other: Eisenia foetida
Endpoint	:	mortality
Exposure period	:	14 day(s)
Unit	:	mg/kg soil dw
NOEC	:	= 7994
LC50	:	> 7994
Method	:	OECD Guide-line 207 "Earthworm, Acute Toxcity Test"
Year	:	1996
GLP	:	yes
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

Result :

Earthworm survival (mean % survival) in the controls met guideline requirements, which validates the test results.

Soil samples loaded at 10,000 mg DIDP/kg soil were analyzed for DIDP at test initiation and termination. The following are the soil analytical results based on the mean of duplicate samples:

Soil Sample	DIDP Conc. Day -1 (mg/kg soil, dry wt.)	DIDP Conc. Day 14 (mg/kg soil, dry wt.)
Snyder Soil	7664	7994
Artificial Soil	8435	9180

DIDP demonstrated no effect on survival in the two soils tested at a soil loading of 10,000 mg/kg soil (dry wt.). The following are the survival results:

Soil Sample	Earthworm Survival*	Mean % Survival
Snyder Soil Control	10,10,10,10,10	100
Artificial Soil Control	10,10,10,10,10	100
Snyder Soil + DIDP	10,10,10,10,10	100
Artificial Soil + DIDP	10,9,10,10,10	98

*10 earthworms were added per replicate. There were five replicates per control and treatment.

Test condition :

Two soils were tested, a natural soil and an artificial soil. Natural soil was obtained from Snyder Research Farm located in Pittstown, NJ, USA, which was managed by Rutgers University. The soil was sieved through a 10 mesh sieve prior to use to remove large particles. Artificial soil was prepared using 70% sand, 20% clay, 10% peat, and CaCO3 to adjust pH.

Test soil was homogenized prior to use by placing soil into 4L size plastic (HDPE) containers and mixing on a jar mill for approximately 15 minutes. After homogenizing, a sample was removed to determine the moisture fraction. The moisture fraction was measured by placing soil into a crystallizing dish and weighing it (initial wt.). The sample and crystallizing dish were then placed in an oven at 100C for 23 hours. After drying and cooling in a desiccator, the final weight of the sample and crystallizing dish was measured.

The water holding capacity of each soil was determined as follows: 25g of

the dried sample was placed into a 100mL glass beaker with 25mL of reverse osmosis water and mixed thoroughly. This slurry was added to a pre-weighed, wetted filter paper and funnel (initial weight = wt. of funnel, wetted paper, + 25 g soil). The filter paper (#113 Whatman 150mm) was wetted with 9mL of reverse osmosis water. The glass funnel measured 10cm top diameter with an approximately 30mm stem. The slurry, filter and funnel were covered with aluminum foil and allowed to stand for 3 hours at which time a final weight was measured. The water holding capacity, expressed in mL water/100g of soil, is the difference between the final and initial weights multiplied by 4 to achieve 100g equivalence.

Treatments were prepared by adding the appropriate amount of test material to a soil sample. The treatment soils were stirred copiously in stainless steel bowls with stainless steel spoons for 15 to 30 minutes and held overnight at room temperature. On day 0, each treatment was divided into 5 replicates. The test chambers were one pint glass canning jars containing approximately 200g of a soil control or treatment and the appropriate amount of hydration water to bring the soils up to 75% of their water holding capacity. The worms were then transferred to randomized test chambers, which were capped with a lid containing a 1/8 inch hole in the center.

Test temperature ranged from 18.2 to 20.6C as measured continuously and recorded by computer for the first 6 days, then measured daily thereafter. Light intensity ranged from 721 to 1185 Lux. Lighting was measured continuously and recorded by computer for the first 6 days, then measured daily thereafter.

Soil pH was measured at test initiation (day 0) of the study. Ten grams of each treatment were mixed with 20mL of distilled water. The pH value of the slurry was measured using a soil pH probe. Soil pH ranged from 6.9 to 7.2.

Observations for worm mortality were performed on all replicate chambers on day 7 and 14. Worms not found were considered dead due to rapid decomposition of worms in soil.

Test substance : CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich. No information on purity, but believed to be 100% commercial product.

Conclusion : DIDP was not lethal to an earthworm at a very high test material/soil loading.

Reliability : (1) valid without restriction
The study was conducted according to the test guideline and there were no significant deviations to the guideline that would suggest the results were questionable. Therefore the study was assessed as valid.

Flag : Critical study for SIDS endpoint
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4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 3160 mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Remark	:	A single 24-hour application of undiluted DIDP (200 and 3160 mg/kg) was applied to abraded rabbit skin under occlusive covering (n = 4). A 14 day observation period was used.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

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Type	:	LD50
Value	:	> 3160 mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	4
Vehicle	:	
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Remark	:	A single 24-hour dermal exposure of undiluted DIDP was applied to the abraded skin of rabbits (4 animals, sex not specified).
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich

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5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella strains TA98, TA100, TA1535, TA1537
Test concentration	:	0, 100, 333, 1000, 3333, 10000 ug/plate
Cycotoxic concentr.	:	high dose was not cytotoxic; otherwise, not specified
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: Ames BN et al. Mutat Res. 31:347-364.
Year	:	1975
GLP	:	no data
Test substance	:	other TS: Disodecyl Phthalate (CAS# 26761-40-0)
Method	:	other: Ames BN et al. Mutat Res. 31:347-364. Positive controls dissolved in DMSO without S9: TA98: 4-nitro-o-phenylenediamine TA100, TA1535: sodium azide TA1537: 9-amino-acridine Positive controls dissolved in DMSO with S9 for all strains: 2-aminoanthracene
Remark	:	Standard plate and preincubation test both with and without metabolic activation (Aroclor induced rat or hamster liver S-9). DIDP was tested at 5 dose levels separated by half-log intervals.
Result	:	Negative; each was done in duplicate.
Test substance	:	Disodecyl Phthalate (CAS# 26761-40-0)

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Type	:	Mouse lymphoma assay
System of testing	:	TK locus of mouse lymphoma cells, L5178Y cell line
Test concentration	:	0.25 to 10 ul/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	other TS: unspecified Disodecyl Phthalate
Remark	:	There was no indication of mutagenic potential for DIDP in the mouse lymphoma assay.
Conclusion	:	The data presented in this report confirm the general lack of genotoxicity for DIDP. Phthalate esters do not contain substructures that would be considered 'alerting' for mutagenicity.

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5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	other: gavage, gavage vehicle: corn oil
Exposure period	:	24, 48, and 72 hours
Doses	:	1250, 2500, and 5000 mg/kg
Result	:	negative
Method	:	other: modification of Heddle et a. Mutat. Res. 123:61-118
Year	:	1983
GLP	:	yes
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Method	:	Modification of Heddle et a. Mutat. Res. 123:61-118. Modifications: 1. 1000 polychromatic erythrocytes were scored for micronuclei per animal. 2. 5 animals per dose/harvest were used
Remark	:	A total of 130 animals were used with 10 animals (5 male and 5 female) randomly assigned to each dose/harvest time. Cyclophosphamide was used as the positive control. It was solubilized in sterile deionized water and administered by oral gavage at 80mg/kg. The positive control animals were euthanized 24hrs. after administration. DIDP was inactive in an in vivo micronucleus test. There were no significant differences between treatment groups and controls for either male or female mice at any dose or collection time.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Conclusion	:	No Clastogenic effects in bone marrow.

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5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gd 6 through 15
Frequency of treatm.	:	daily
Duration of test	:	gestation day 21
Doses	:	100, 500, 1000 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	500 mg/kg bw
NOAEL teratogen.	:	1000 - mg/kg bw

Method	:	Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	:	1981
GLP	:	yes
Test substance	:	other TS: CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Remark	:	The result indicate that DIDP was neither a selective developmental toxicant nor an embryotoxic agent.
Result	:	Maternal toxicity was indicated by reductions in body weight gain and food consumption. There was no evidence of malformations or fetal toxicity.
Test substance	:	CAS #68515-49-1; 1,2-benzenedicarboxylic acid, di-C9,C10 and C11 branched alkyl ester, C10 Rich
Reliability	:	(1) valid without restriction

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5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT